2-Methylphenanthrene

2531-84-2 | DTXSID1025649

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.72e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.29e-01

Confidence level: 6.43e-01

Nearest Neighbors from the Training Set

Image not found
7-Methylquinoline
Measured: 5.34e-06
Predicted: 1.73e-02

Image not found
2,6-Toluenediamine
Measured: 1.50e-05
Predicted: 8.84e-04

Image not found
9,10-Dihydrophenanthrene
Measured: 4.00e-05
Predicted: 2.90e-04

Image not found
Dihexyl phthalate
Measured: 1.21e-04
Predicted: 7.80e-06